Neglected Opacity Issues

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Neglected Opacity Issues

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Oscillator Strengths

Conservation of Oscillator Strength:

The Thomas-Reiche-Kuhn sum rule should be used to check one-electron sequences ($\Sigma_m f_{nm} = 1$) and Z-electron atoms ($\Sigma_{nm} f_{nm} = Z$).

Continuity of Oscillator Strength:

In a one-electron sequence the sum rule is continuous from bound-bound to bound-free absorption. See Fano and Cooper Rev. Mod. Phys. **44**, 441 (1968).

Completeness of Species Considered

- Test For the Formation of Molecules:

While it may not be of interest to calculate molecular contributions to opacity at low temperatures, tests should be included to warn the user that the opacity lacks molecular contributions, and list the molecules that may form from the mixture of elements considered.

Completeness of Species Considered (continued)

- Minimization of the Gibbs free energy of formation for species of chemical elements and compounds in their gas and condensed phases is general, elegant, powerful, and guarantees conservation of matter. This method automatically includes reactions of dis-proportionation and reactions involving condensed phases.

$$G = \Sigma_{p=1}^{q+s+1} \Sigma_{i=1}^{m_p} n_{pi} (\Delta G_{pi} R_o T \ln a_{pi}),$$

where p represents a gas phase, q the number of condensed phase solutions, s the number of pure condensed phases, m_p the number of species in each phase, n_{pi} the number of moles of species i in phase p, and a_{pi} the activity of species i in phase p.

Completeness of Species Considered (continued)

- Heavy Element Impurities:

It is absolutely essential that impurities be included in the calculation of mixtures. This is particularly true if the impurities are from elements with a higher Z.

Uncertainties in Opacities

- Uncertainties in Models, Methods, and Calculations:

Arise from the need to know atomic and molecular structure, stages of ionization and dissociation, level populations, spectral line shapes, and plasma interactions.

- Sources of Uncertainties:

1. Physical process
2. Chemical (elemental) abundances
3. Mathematical procedures.

Physical Process

Sources include approximations in the model of the atom or molecule used to describe the absorption and scattering processes:
Configuration interaction
Line broadening
Line shapes and line wings
Pressure balance
Collective effects
Charge conservation
Element conservation in phase transitions

Chemical Abundances

The usual approximation is the abbreviation of the elemental, molecular, and ionic composition of a medium to its “most important” constituents.

Some very underabundant species may have a line or band spectrum in an important region where the extinction coefficients of the most abundant species are very small.

Spectra of major and minor species should always be inspected.

Mathematical Procedures

Primarily iterative convergence procedure, fits to tabular data, limits imposed by electronic computers (e.g., accidentally cancellation of two nearly equal numbers).

Completeness of Processes Considered

Contribution of Plasmons to Opacity (Keady et al., 1990):
Plasmon = quantum of charge-density oscillation in a plasma.
When an x-ray interacts with an electron in a plasma, the recoil energy of the electron may remove it from the collective modes of the plasma, generating density fluctuations and creating plasmons. This influences Compton scattering. From energy conservation

$$h\nu + \gamma mc^2 = h\nu' + h\nu_p + \gamma' mc^2\ , \qquad \gamma = [1 - (\mathrm{v}/c)^2]^{-1/2}\ .$$

ν = incident photon, v = initial velocity of electron, m = electron mass, ν_p = plasma frequency. The plasmon energy is the binding energy of the electron to the plasma.

Plasmons (continued)

From momentum conservation

$$(h\nu/c) + \gamma m\mathrm{v}\cos\theta = (h\nu'/c)\cos\Theta + \gamma' m\mathrm{v}'\cos\theta'$$

$$\gamma m\mathrm{v}\sin\theta = -(h\nu'/c)\sin\Theta + \gamma' m\mathrm{v}'\sin\theta'$$

Angles are relative to the incident photon. θ, θ' = initial and final direction of electron, Θ = direction of photon. The plasmon is heavy compared to electron. Momentum transfer to plasma is negligible.

$$h\nu' = \frac{(h\nu_p)^2 - 2\gamma h\nu_p mc^2 - 2h\nu h\nu_p + 2\gamma h\nu mc^2 - 2\gamma h\nu mc\mathrm{v}\cos\theta}{2h\nu - 2\gamma mc\mathrm{v}\cos(\theta + \Theta) - 2h\nu\cos\Theta - 2h\nu_p + 2\gamma mc^2} .$$

The differential cross section for excitation is

$d\sigma_P/d\omega = (e^2/mc^2)^2\,[1 - (1/2)\sin^2\Theta]\,S(\boldsymbol{k})$, $S(\boldsymbol{k}) = h\boldsymbol{k}^2/(8\pi^2 m\nu_p)$

$h\boldsymbol{k}/(2\pi)$ = momentum transfer of photon to electron.

Plasmons (continued)

Substituting $h\nu'$ and integrating gives for $\nu >> \nu_p$ the total plasma interaction cross section

$$\sigma_P = (8\pi/3)\,(e^2/mc^2)^2\,(h\nu)^2/(2mc^2 h\nu_p)\;.$$

$$\sigma_P = (2\pi/3)\,\alpha^6\,a_o^2\,(h\nu)^2/(h\nu_p)\;,\quad \text{in Rydberg units.}$$

For keV x-rays and typical plasma conditions, this cross section is same order magnitude as the Compton cross section.

Plasmon effects can be important at high densities, where,however, free-free absorption may dominate over scattering.

The cross sections must be multiplied by the form factors F_{inc} and F_{coh} for incoherent and coherent scattering, respectively.

Special Cases

- Failure to Attain LTE:

For heavier elements, LTE conditions may not be attainable at high temperatures and low densities because radiative deexcitation may be faster than collisional excitation.

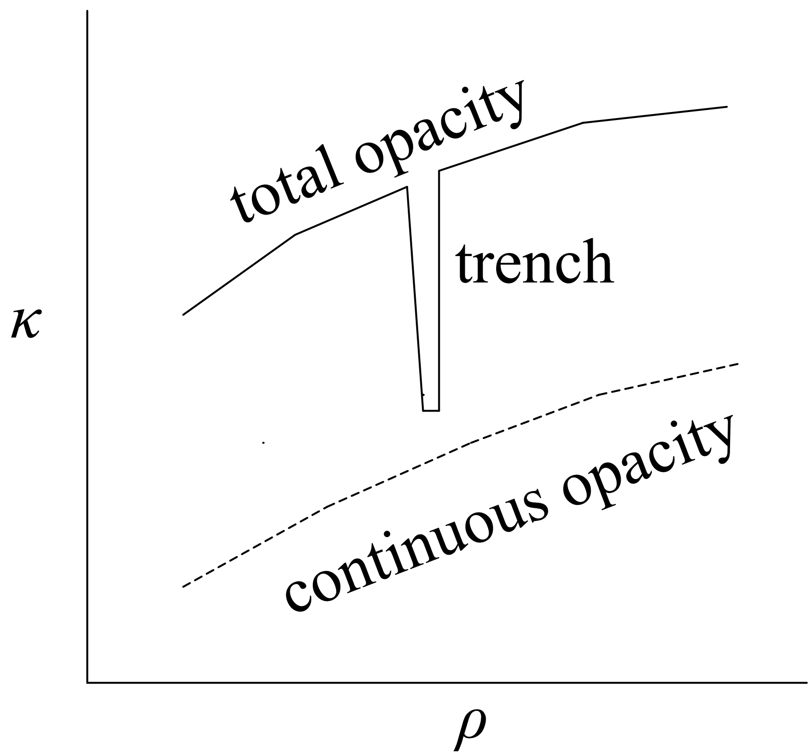
Special Cases (continued)

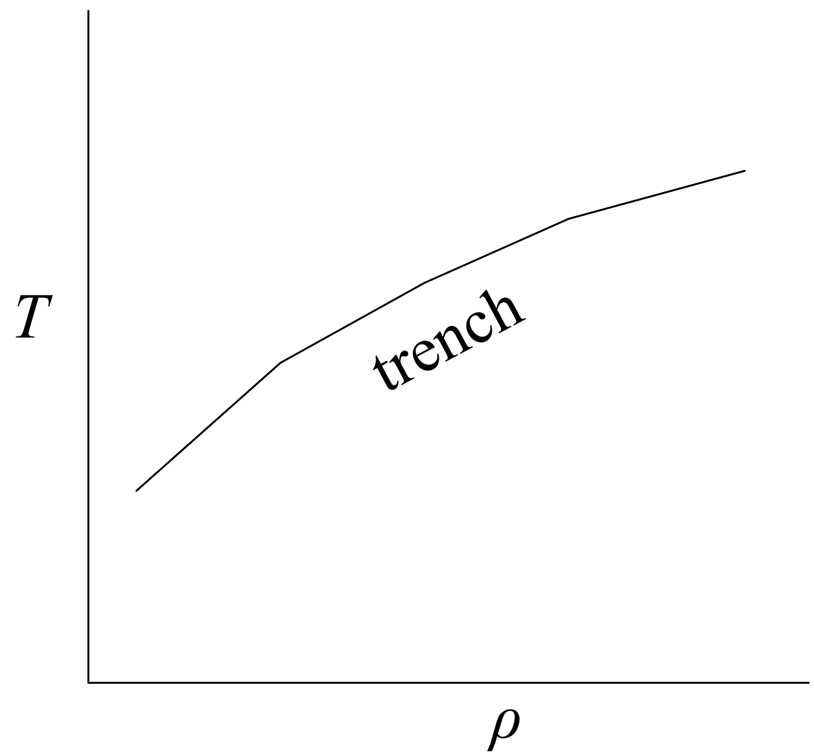
- Opacity Trenches:

Partially filled shells bring about many electron configurations and many different ways for electrons to couple. The result is a plethora of overlapping spectral lines. For some elements temperature-density regions exist in which the ion structure is dominated by closed shells. There, the number of possible electron configurations and couplings are severely limited when compared to neighboring regions with more than one electron (or electron hole) relative to the closed shells. As a result the line spectrum is sparse and the opacity is drastically reduced. The temperature-density regions where this opacity reduction occurs is very narrow, i.e., like a trench.

Special Cases (continued)

Opacity Trenches:





Designing Opacities to Meet Requirements

Designing materials to meet opacity requirements:
For example:
High opacity from low-Z elements.
Opacities that block a photon energy range over a certain T - ρ range.

Laboratory Experiments

Validation of opacity codes and verification of opacity calculations are very important. One has to keep in mind that opacity calculations are complex, but individual processes can be checked independently. Laboratory experiments are complex, but individual processes cannot be checked independently.

Difficulties with laboratory experiments include:

1. Attainment of LTE
2. T and ρ determination
3. T and ρ gradients
4. Edge effects
5. Back lighting
6. Plasma impurities

Laboratory experiments can provide supporting evidence for opacity calculations.

Benchmark Calculations

Opacity calculations are based on many processes. Most of these processes are calculated using different models, different wave functions, disjointed processes (e.g., line wings vs. underlying continuum, absorption vs. scattering, etc.). Sometimes not even The elemental composition is consistent across phase transitions (e.g., with rising temperature from a dusty atmosphere – molecular gas – atomic gas – plasma).
A detailed benchmark calculation for a pure plasma should be carried out (perhaps in conjunction with an opacity experiment)**.**